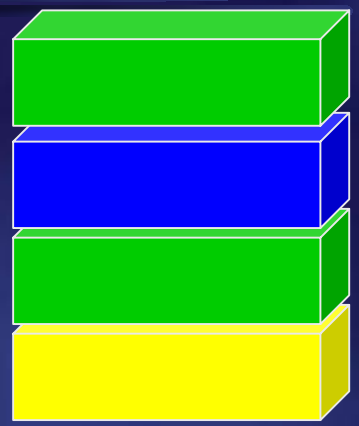
Towards a Deep Microscopic Understanding of Ferroelectric Alloys

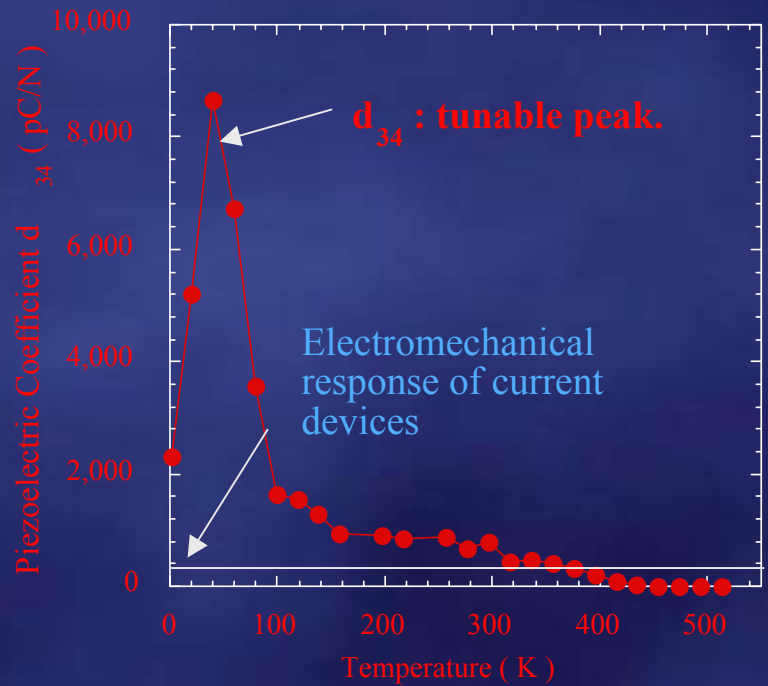
Laurent Bellaiche, University of Arkansas, DMR Award#9983678

If we can fundamentally understand ferroelectric alloys, we can take the necessary steps to increase the desired response of these alloys. Using ab-initio methods, we have found that when certain alloys are optimally ordered, new structural phases can occur and electromechanical responses of the crystal can be improved by a factor of more than ten (A. M. George *et al.* ***Nature***, **413**, 54-57 (2001)). These are the responses exploited by listening and communications devices. An added feature of this ordering is the ability to tune the peak response to specified operating conditions such as temperature. This finding means we can drastically improve the response of devices, even in inhospitable environments such as space and deep sea. This could significantly advance the quality of devices (ultrasound, accelerometers, actuators etc.) used in industry. Interestingly, these findings can be understood by simple electrostatic arguments.

Atomic Ordering in $Pb(Sc_{0.5}Nb_{0.5})O_3$



Electro - mechanical response



Towards a Deep Microscopic Understanding of Ferroelectric Alloys
Laurent Bellaiche, University of Arkansas, DMR Award#9983678

Educational:
1 undergraduate,
5 graduate students,
1 research associate,
1 scientific visitor from Spain.
The mentioned above personnel worked on this project.

Collaborators:
- Benjamin P. Burton (NIST, MD)
- Eric Cockayne (NIST, MD)
- Ronald E. Cohen (Carnegie Inst. of Washington, DC)
- Alberto Garcia (Univ. Del Pais Vasco, Spain)
- Jorge Iniguez (Rutgers University, NJ)
- David Vanderbilt (Rutgers University, NJ)

Brief summary of outreach activities:
1. Research Experience during Summer 2002 for an African-American undergraduate student of Xavier University (LA)
2. Three Master degrees obtained in Fall 2001 by students of University of Arkansas (including one belonging to an underrepresented minority group)
3. Research Experience during summer 2000, 2001, 2002 for graduate students eager to learn ab-initio techniques and ferroelectrics, in addition to their normal courses
4. Collaboration with national laboratories and other Universities involving graduate students

Figure 2. ***Photo of PI's group taken in Spring 2002. From left to right: Alireza Akbarzadeh, Laurent Bellaiche, Igor A. Kornev, Horace Crogman, Aaron George, Derrick Johnson, Abdullah Al-Barakaty, David Sichüga***

5. Design and Teaching of advanced solid state physics I and II graduate courses. Homeworks dealing with ferroelectrics, as well as reports on published articles on ferroelectrics, were often assigned to "put in practice" concepts (learnt in class) on crystallography and ionic vibrations in solids
6. Development and maintenance of a web site (describing the research activities of the PI's group) by the graduate student entirely sponsored by the NSF grant
7. Advertisement of the research findings in local, regional, national and international meetings, as well as in local and regional newspapers.